A computer implemented method for configuring the molecular structures derived from reactant molecules into a standardized representative conformation enabling comparison between the structures of shape related properties, comprising the following steps:

a)   defining topomeric alignment rules;

b)   obtaining, or generating from two dimensional (2D) structural information, the three dimensional (3D) configuration of the molecular structures represented by the three dimensional coordinates of the atoms *—CONCORD* comprising the structures; and

c)   repositioning the relative positions of atoms in the structures by adjusting torsions according to the topomeric alignment rules

wherein a single, consistent, and unambiguous aligned topomeric conformation is produced for each structure.

for record only as discussion